Course Structure
lecturer: Maria Datcheva

Starts: 15th of October  
Ends: 19th of December

This course is composed of

14 lectures - 11 seminars – 2 project

compressed to

10 lectures – 6(7) seminars – 1 project

Book

Wei-Fan Chen, Atef F. Saaleb

Constitutive Equations for Engineering Materials
Constitutive models - Introduction

Course Structure

This module of lecture material is assigned one short set of homework questions.

There will be 1 project to be elaborated and presented

2 teams, 2 topics
(recent scientific articles close to your professional topic)

The material in this module will also be covered in the final exam

- 19\textsuperscript{th} of December, 2007

or

- ?\textsuperscript{th} of January, 2008
Constitutive models - Introduction

Time table
(flexible arrangement)

• Lectures
  – Monday: 15:15 - 16:45 (Coudraystrasse 11c, room 101)

• Seminars
  – Wednesday: 13:30 - 15:00 (Coudraystrasse 11c, room 101)
  – October 31 – Reformationstag (civic holiday in Thuringia)
    1517, Martin Luther

Last seminar is meant for preparation to the exam
Constitutive models – Introduction – rational mechanics

i.e., conceptual and mathematical mechanics
Truesdell, Noll, etc

general laws
The modern mechanical theories regard bodies as subject to general laws applying to all types of materials, laws that characterize geometry of space, time and motion, the structure of material bodies, the nature of systems of forces and the relation of forces to motion.

special laws
Mechanics uses the term constitutive assumption to refer to the special laws for particular materials, since these laws reflect assumptions about the constitution of the material.

Mechanical practice depends critically on these special laws.

Constitutive assumptions – relations – laws – equations are the TOPIC of this lecture course
Constitutive models – Introduction – rational mechanics

Events, Time and Space

3D space (i.e. with Cartesian coordinate system) + $t$
reference system related to the universe of events: $\Phi(x,t)$

Bodies
point mass; rigid bodies; strings, rods, streams (1D); membranes and shells (2D)
fluids and solids (3D)

Forces, Mass
force systems - each force system induces two subsidiary force systems:
internal forces between separate parts of a body (gravity...), and
external forces exerted by the exterior of a body on its parts (applied F, friction...).

Motion
Standard mechanics assumes continuity of the first two derivatives of motions
and frames of reference. It is related to the configuration and deformation of the
body (+ axiom of impenetrability )

constitutive relations
Constitutive models – Introduction – rational mechanics

Constitutive relations – laws – theory
is based on the following axioms

Axiom 1  Deterministic principle:
stress state at configuration body-point \( X \) at moment \( t \)
is determined by the prehistory of the body motion up
to the moment \( t \)

\[ \Rightarrow \text{past and the present configurations of the body determine the stress field} \]
that acts on the present configuration

Axiom 2  Principle of the local effect (of locality)

Axiom 3  Independence of the reference system
\[ \Rightarrow \text{material properties and constitutive laws, respectively do not depend on the} \]
choice of the observer (invariance regarding orthogonal transformations).
This means constitutive mappings are not form-invariant with respect to changing the state of motion of matter, but of course they are covariant (form-invariant) with respect to changing the observer.

... theory with theorems, lemmas, etc
Constitutive relations being ideal and approximation to the real material properties are build within the theory that have strong axiomatic structure and they are not simple fit to the observed experimental data. This is a direct consequence from that constitutive laws are part of the mathematical models of the universe processes.

This is where the constitutive field theory generation process has to be invoked in terms of the determination of constitutive functionals that usually relate the first member (stress) of the conjugate state variable pair with the second one (strain) according to the constitutive law.
Constitutive models – Introduction – engineering application

**Engineering Problem**

**Boundary and initial value problem**
geometry, applied constrains, forces etc.

Starting point for deriving partial differential equations (PDE) lies in the conservative laws of physics

- Conservation of mass (Continuity equation)
- Conservation of energy (Equation of equilibrium/ motion)

**Add constitutive relationships** (stress-strain relationships)

SOLVE the PDE – BVP numerically: FE; FD; FV etc

PREDICTIONS

nonlinear PDE, geometrical nonlinearity: analytical solution rarely possible
Constitutive models – Introduction – engineering application

Suggestions on developing and using constitutive models

• The more complex (or ill-defined) the constitutive model, the more likely it is to run into numerical ill-conditioning, convergence and instability problems.

• Models must be “simple but not simpler” (following Einstein philosophy).

• It is essential to determine at the outset of the analysis what type of response results are of greatest importance to be recovered by the model (aspect and region).

• Achieving accuracy with respect to a given aspect of the response for a given boundary value problem does not require and/or ensure that all aspects are modelled accurately, e.g., accurate modelling of failure may not be achieved if only small displacements are considered in the model, time dependent effects may be discarded, etc.

• It is of paramount importance to have good estimates of the initial values of the constitutive model parameters (material and model parameters) => need of model calibration (back analysis), verification and validation.

Boundary and initial value problem

geometry, applied constraints, forces etc. Starting point for deriving partial differential equations (PDE) lies in the conservative laws of physics

Conservation of energy

(Equation of equilibrium/motion)

Add constitutive relationships (stress-strain relationships)

Conservation of mass

(Continuity equation)

Solve the PDE – BVP numerically: FE; FD; FV etc.
Constitutive models – Introduction – engineering application

Engineering Problem

Suggestions on developing and using constitutive models

- Start with simple constitutive model (linear elastic or comparable).
- Avoid the “finite elephant” syndrome where the model one is running has completely taken over the modeller, or where the modeller has completely lost control of the model.

Conservation of mass (Continuity equation)

Conservation of energy (Equation of equilibrium/motion)

Add constitutive relationships

Predictions

nonlinear PDE, geometrical nonlinearity: analytical solution rarely possible

Marte Gutierres
This course will draw heavily on previous mathematics:

- **calculus** (differential, integral);
- **partial differential equations**; boundary value problems;
- **tensor algebra** (basics)

The use of **tensor** notations is commonplace in the current literature when **constitutive** equations are described → **basic knowledge is essential!**

**Vectors** → dot product, cross product, grad, div, curl, angle between vectors.

**Tensors** → 2nd and 4th order symmetric tensors, eigenvalues, eigenvectors, invariants.

**Scalar, vector and tensor fields** → polynomial, homogeneous, potential functions etc.
Constitutive models – Introduction – some maths and notations

- **Scalars** – objects that have only a magnitude
- **Vectors** – objects that possesse both magnitude and direction

\[
a(a_1, a_2, a_3); \ a = a_i e_i
\]

**notation:** equal indices = summation

**scalar (dot) product:** \( a \cdot b = a_i b_i \)

**cross (outer) product:**
\[
c = a \times b = \begin{vmatrix} e_1 & e_2 & e_3 \\ a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{vmatrix} = \begin{pmatrix} a_2 b_3 - a_3 b_2 \\ a_3 b_1 - a_1 b_3 \\ a_1 b_2 - a_2 b_1 \end{pmatrix}
\]

**prove:** \( (a \cdot b) c = a (b \cdot c) \)

*Vectors and matrices*
Constitutive models – Introduction – some maths and notations

Scalar and vector fields: temperature velocity
(scalar/vector function)
\[ T(x_1, x_2, x_3, t) \quad \nu(x_1, x_2, x_3, t) \]

Gradient:
\[ G_i = \frac{\partial \Phi}{\partial x_i} = \Phi_{,i} = \text{grad}_i \Phi = \nabla_i \Phi \]
\[ \nabla \Phi = e_i \frac{\partial \Phi}{\partial x_i} = \text{grad} \Phi \]

Prove: \( \Phi(x_1, x_2, x_3, t): \frac{\partial \Phi}{\partial x_i} = e_i \cdot \nabla \Phi \)

Divergence:
\[ \text{div} \nu = \nabla \cdot \nu \quad \text{Prove:} \quad \nabla \cdot \nu = \nu \cdot \nabla \]

Curl (rot):
\[ \text{curl} \nu = \nabla \times \nu \]

Laplacian:
\[ \Delta \Phi = \nabla \cdot \nabla \Phi = \Phi_{,ii} \]
*summation convention
Coordinate transformation

\[ \xi \rightarrow \xi' \]

\[
x_1' = \alpha_{11}x_1 + \alpha_{12}x_2 + \alpha_{13}x_3 = \alpha_{ij}x_j \\
x_2' = \alpha_{2j}x_j \\
x_3' = \alpha_{3j}x_j \\
\Rightarrow \quad x_i' = \alpha_{ij}x_j
\]

\[
\alpha_{ij} = \cos(x'_i, x_j) = \frac{\partial x'_i}{\partial x_j} = \cos(e'_i, e_j) = e'_i \cdot e_j
\]

\[ x' = R x \quad R_{ij} = \alpha_{ij} - \text{rotational matrix} \]

Tensor of 2nd order (definition): \[ T'_{ij} = \alpha_{ik} \alpha_{jl} T_{kl} \]

Orthogonal condition: \[ \alpha_{ij} \alpha_{il} = \delta_{jl} - \text{Kronecker delta} \]
Constitutive models – Introduction – some maths and notations

Permutation symbol:

\[ \varepsilon_{ijk} = \frac{1}{2} (i - j)(j - k)(k - i) \]

Kronecker delta:

\[ \delta_{ij} = \begin{cases} 
1 & \text{if } i = j \\
0 & \text{if } i \neq j 
\end{cases} \]

\[ \mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij} \quad \text{(orthogonal basis)} \]

Decomposition of matrix (and tensor of 2nd order):

\[ A_{ij} = \frac{1}{2} (A_{ij} + A_{ji}) + \frac{1}{2} (A_{ij} - A_{ji}) \]

symmetric \hspace{1cm} \text{anti-symmetric/screw symmetric}
Constitutive models – Introduction – some maths and notations

**Indicial notations – summation convention**

A subscript appearing twice is summed from 1 to 3

\[ a_i b_i = a_1 b_1 + a_2 b_2 + a_3 b_3 \]

\[ D_{ii} = D_{11} + D_{22} + D_{33} \]

\[ \alpha_{ij} x_j = x_i \]

\[ a_{ij} a_{ij} = a_{11}^2 + a_{22}^2 + a_{33}^2 + a_{12}^2 + a_{21}^2 + a_{23}^2 + a_{32}^2 + a_{13}^2 + a_{31}^2 \]

**Comma – subscript convention**

\[ \frac{\partial \phi}{\partial x_i} = \phi_i = \text{grad}\phi; \quad \frac{\partial v_i}{\partial x_i} = \text{div}\mathbf{v}; \quad \frac{\partial v_i}{\partial x_j} = v_{i,j}; \]

\[ \frac{\partial^2 v_i}{\partial x_j \partial x_k} = v_{i,jk} \]
Constitutive models - Introduction

Traction, stress and equilibrium

Stress tensor

Deformation / strain tensor

Tensor's invariants (2nd order)
Constitutive models - Introduction

Pilot test (name, e-mail, main topic of interest):

1. \[ f(x_1, x_2, x_3) = 3x_1 + x_1 e^{x_2} + x_1 x_2 e^{x_3} \]

(a) \( \text{grad} \ f = \)?  
(b) \( \text{grad} \ f(3, 1, 0) = \)?

2. Is the equation of motion a constitutive equation?

3. Give the name of at least one constitutive law you know.

3. For the tensor \( T_{ij} \) it holds \( T_{ij} = -T_{ji} \) \( \forall i, j = 1, 2, 3 \). Write the tensor \( T_{ij} \) as a matrix. Give the rank (order) of the tensor \( T_{ij} \).

4. In 2D a coordinate transform \( x_i \rightarrow x'_i \) is defined with the angle between \( x_1 \) and \( x'_1 \) equal to \( \pi/2 \). Give the rotational matrix \( \alpha_{ij} \).